

Author index to volume 273

- Al-Omari, A.K., R. Reininger and D.L. Huber, Temperature effect on the ionization potential line-shape of NO doped into dense gaseous argon 273 (1997) 402
- Alonso, J.A., see Marcos, P.A. 273 (1997) 367
- Anderson, D.T., see Schwartz, R.L. 273 (1997) 18
- Asai, K., see Yamaki, T. 273 (1997) 376
- Bahou, M., L. Schriver-Mazzuoli, C. Camy-Peyret and A. Schriver, Photolysis of ozone at 693 nm in solid oxygen. Isotopic effects in ozone reformation 273 (1997) 31
- Barnett, R.N., Z. Sun and W.A. Lester Jr., Fixed-sample optimization in quantum Monte Carlo using a probability density function 273 (1997) 321
- Bartels, L., G. Meyer and K.-H. Rieder, Basic steps involved in the lateral manipulation of single CO molecules and rows of CO molecules 273 (1997) 371
- Bauer, C., see Hubrich, M. 273 (1997) 259
- Bauschlicher, Jr., C.W., Displacement energies for nanorods 273 (1997) 195
- Berden, G., see Jongma, R.T. 273 (1997) 147
- Blackwell, M., see Ludowise, P. 273 (1997) 211
- Bollati, R.A. and J.C. Ferrero, Quasiclassical trajectory simulations of the collisional deactivation of vibrationally excited $\text{HgBr}(\text{B}^2\Sigma, v=52)$ by N_2 273 (1997) 129
- Bower, P.V., see Hohwy, M. 273 (1997) 297
- Bréchnignac, P., see Douin, S. 273 (1997) 389
- Brenton, A.G., see Lock, C.M. 273 (1997) 1
- Brutschy, B., see Lembach, G. 273 (1997) 421
- Bykov, L., see Lifshitz, E. 273 (1997) 381
- Camy-Peyret, C., see Bahou, M. 273 (1997) 31
- Cha, Y.-H., Y. Furukawa, M. Tasumi, T. Noguchi and T. Ohnishi, Photoinduced infrared absorptions from conjugated polymers with nondegenerate ground states 273 (1997) 159
- Chang, T.-C., see Chiang, C.-C. 273 (1997) 153
- Chen-Esterlit, Z., see Lifshitz, E. 273 (1997) 381
- Chen, Y., see Ludowise, P. 273 (1997) 211
- Chiang, C.-C., C.-Y. Mou and T.-C. Chang, Photoreaction of neutral 9-aminoacridine in glycerol:water glass characterized by satellite holes and antiholes 273 (1997) 153
- Clary, D.C., see Jeffrey, S.J. 273 (1997) 55
- Cox, S.F.J., I.D. Reid, K.L. McCormack and B.C. Webster, Muonium radical formation in elemental sulphur 273 (1997) 179
- Creve, S. and M.T. Nguyen, On the geometry and inversion process of $\text{PF}_3^+(\tilde{\text{X}}^2\text{A}_1)$ 273 (1997) 199

- Danovich, D., see Harvey, J.N. 273 (1997) 164
D'Arco, P., see Tappero, R. 273 (1997) 83
De Natale, P., L. Lorini, M. Inguscio, G. Di Lonardo and L. Fusina, High-sensitivity detection of the rotation spectrum of HCl in the $v = 1$ state by tunable FIR spectroscopy 273 (1997) 253
Deng, W.-Q., see Huang, J.-H. 273 (1997) 205
Diestler, D.J., see Schoen, M. 273 (1997) 296
Di Lonardo, G., see De Natale, P. 273 (1997) 253
Doktorov, A.B., see Neufeld, A.A. 273 (1997) 311
Dolg, M., see Yu, M. 273 (1997) 329
Douin, S., S. Piccirillo and P. Bréchnignac, Solvation of charge in aromatic/noble gas Van der Waals clusters 273 (1997) 389
Dressler, S. and W. Thiel, Anharmonic force fields from density functional theory 273 (1997) 71
Duncan, M.A., see Knight, A.M. 273 (1997) 265
Duppen, K., see Steffen, T. 273 (1997) 47
Dupre, P., see Li, H. 273 (1997) 272
Erman, P., A. Karawajczyk, E. Rachlew-Källne, M. Stankiewicz, K. Yoshiki Franzén, P. Sannes and L. Veseth, Photoionization processes in NO in the threshold region 273 (1997) 239
Fan, H.-J., C.-W. Liu and M.-S. Liao, Geometry, electronic structure and magnetism of small Co_n ($n = 2-8$) clusters 273 (1997) 353
Fan, K.-N., see Wang, W.-N. 273 (1997) 337
Ferrero, J.C., see Bollati, R.A. 273 (1997) 129
Fries, P.H., see Richardi, J. 273 (1997) 115
Furukawa, Y., see Cha, Y.-H. 273 (1997) 159
Fusina, L., see De Natale, P. 273 (1997) 253
Geipel, N.J.M. and B.A. Heß, Scalar-relativistic effects in solids in the framework of a Douglas-Kroll transformed Dirac-Coulomb Hamiltonian 273 (1997) 62
Glushkov, V.N., Asymptotic method of building restricted open-shell wavefunctions satisfying the generalized Brillouin's theorem 273 (1997) 122
Green, W.H., see Tozer, D.J. 273 (1997) 183
Haarer, D., see Zilker, S.J. 273 (1997) 232
Han, K.-L., see Huang, J.-H. 273 (1997) 205
Handy, N.C., see Tozer, D.J. 273 (1997) 183
Hartwigsen, C., see Witschel, W. 273 (1997) 304
Harvey, J.N., D. Schröder, W. Koch, D. Danovich, S. Shaik and H. Schwarz, Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations 273 (1997) 164
Hashimoto, T., K. Hirao and H. Tatewaki, Contracted or uncontracted polarization functions? Comment on Dunning's correlation-consistent basis sets 273 (1997) 345
He, G.-Z., see Huang, J.-H. 273 (1997) 205
Herbich, J. and A. Kapturkiewicz, Electronic and molecular structure of charge transfer singlet states: 4-(9-anthryl)julolidine and 4-(9-acridyl)julolidine 273 (1997) 8
Heß, B.A., see Geipel, N.J.M. 273 (1997) 62
Hirao, K., see Hashimoto, T. 273 (1997) 345
Hohwy, M., P.V. Bower, H.J. Jakobsen and N.C. Nielsen, A high-order and broadband CRAMPS experiment using z -rotational decoupling 273 (1997) 297
Honda, Y., M.-B. Song and M. Ito, Current oscillations during the oxidation of formic acid on Pt(100) as studied by in situ time-resolved infrared reflection absorption spectroscopy 273 (1997) 141

- Hong, S.D. and M.S. Jhon, Calculation of excess free energy from the averaged effective acceptance ratio for the Lennard-Jones fluid and the inverse twelve fluid 273 (1997) 79
- Huang, J.-H., K.-L. Han, W.-Q. Deng and G.-Z. He, Theoretical studies of the decyclization/cyclization of the C_6H_5 radical 273 (1997) 205
- Huber, D.L., see Al-Omari, A.K. 273 (1997) 402
- Hubrich, M., C. Bauer and H.W. Spiess, Magic-angle spinning electron paramagnetic resonance spectroscopy 273 (1997) 259
- Ibuki, T., see Tokue, I. 273 (1997) 247
- Inguscio, M., see De Natale, P. 273 (1997) 253
- Ishigure, K., see Yamaki, T. 273 (1997) 376
- Ito, M., see Honda, Y. 273 (1997) 141
- Ito, O., see Watanabe, A. 273 (1997) 227
- Itoh, T., M. Yamaji and H. Shizuka, Emission properties of 1,4-anthraquinone 273 (1997) 397
- Iwata, S., see Li, Y. 273 (1997) 91
- Iwata, S., see Wang, W.-N. 273 (1997) 337
- Jakobsen, H.J., see Hohwy, M. 273 (1997) 297
- Jasny, J. and J. Sepiol, Single molecules observed by immersion mirror objective. A novel method of finding the orientation of a radiating dipole 273 (1997) 439
- Jasny, J., see Sepiol, J. 273 (1997) 444
- Jeffrey, S.J., S.C. Smith and D.C. Clary, Calculation of the vibrational spectral density of NO_2 via density correlation functions 273 (1997) 55
- Jhon, M.S., see Hong, S.D. 273 (1997) 79
- Jongma, R.T., G. Berden, T. Rasing, H. Zacharias and G. Meijer, Scattering of vibrationally and electronically excited CO molecules from a LiF(100) surface 273 (1997) 147
- Jouart, J.P., see Zhang, X. 273 (1997) 416
- Kapturkiewicz, A., see Herbich, J. 273 (1997) 8
- Karawajczyk, A., see Erman, P. 273 (1997) 239
- Kato, T., see Matsushita, M. 273 (1997) 291
- Kawamura, T., Y. Miyazaki and M. Sorai, Heat capacity and crystal polymorph of the organic charge-transfer complex, tetrathiafulvalene-*p*-chloranil 273 (1997) 235
- Keller, J., see Sepiol, J. 273 (1997) 444
- Knight, A.M., A. Stangassinger and M.A. Duncan, Photoionization spectroscopy of Au-Ar 273 (1997) 265
- Koch, W., see Harvey, J.N. 273 (1997) 164
- Kodaira, T., see Watanabe, A. 273 (1997) 227
- Kong, W., see Li, H. 273 (1997) 272
- Krienke, H., see Richardi, J. 273 (1997) 115
- Leblanc, R.M., see Shao, L. 273 (1997) 37
- Lembach, G. and B. Brutschy, Mass analyzed threshold ionization of chlorobenzene and chlorobenzene $\cdot Ar_1$ 273 (1997) 421
- Lester, M.I., see Schwartz, R.L. 273 (1997) 18
- Lester Jr., W.A., see Barnett, R.N. 273 (1997) 321
- Li, H., P. Dupre and W. Kong, Degenerate four wave mixing and laser induced fluorescence of pyrazine and pyridazine 273 (1997) 272
- Li, Y. and S. Iwata, Potential energy surfaces of the ground and low-lying states of HCCS and NCS: CASSCF, MRCI and CCSD(T) studies 273 (1997) 91

- Liao, M.-S., see Fan, H.-J. 273 (1997) 353
- Lichanot, A., see Tappero, R. 273 (1997) 83
- Lifshitz, E., L. Bykov, M. Yassen and Z. Chen-Esterlit, The investigation of donor and acceptor states in nanoparticles of the layered semiconductor PbI_2 273 (1997) 381
- Liu, C.-W., see Fan, H.-J. 273 (1997) 353
- Liu, X., see Zhang, X. 273 (1997) 416
- Lock, C.M., A.G. Brenton and D. Mathur, High-resolution ion translational energy spectrometry of C_{60} . Excitation of singlet and triplet states in collisions with H^+ and H_2^+ 273 (1997) 1
- Long, P., see Lopez-Martens, R. 273 (1997) 219
- Lopez-Martens, R., P. Long, D. Solgadi, B. Soep, J. Syage and Ph. Millie, A time-resolved photoelectron study of the double excited-state proton-transfer reaction in 7-azaindole dimer 273 (1997) 219
- López, M.J., see Marcos, P.A. 273 (1997) 367
- Lorini, L., see De Natale, P. 273 (1997) 253
- Ludowise, P., M. Blackwell and Y. Chen, Femtosecond time-resolved mass and photoelectron spectroscopic study of OCIO photodissociation. Coherent energy transfer in a stepwise reaction 273 (1997) 211
- Marcos, P.A., M.J. López, A. Rubio and J.A. Alonso, Thermal road for fullerene annealing 273 (1997) 367
- Martin, J.M.L., Benchmark ab initio calculations of the total atomization energies of the first-row hydrides AH_n ($A = \text{Li}-\text{F}$) 273 (1997) 98
- Marx, D., M. Sprik and M. Parrinello, Ab initio molecular dynamics of ion solvation. The case of Be^{2+} in water 273 (1997) 360
- Mary, G., see Zhang, X. 273 (1997) 416
- Mathur, D., see Lock, C.M. 273 (1997) 1
- Matsushita, M. and T. Kato, Nuclear quadrupole resonance of ^{139}La around Pr^{3+} doped in LaF_3 . Raman heterodyne detection using optical transition of Pr^{3+} ions 273 (1997) 291
- McCormack, K.L., see Cox, S.F.J. 273 (1997) 179
- Meijer, G., see Jongma, R.T. 273 (1997) 147
- Meyer, G., see Bartels, L. 273 (1997) 371
- Millie, Ph., see Lopez-Martens, R. 273 (1997) 219
- Miyazaki, Y., see Kawamura, T. 273 (1997) 235
- Molin, Yu.N., see Tadjikov, B.M. 273 (1997) 25
- Mou, C.-Y., see Chiang, C.-C. 273 (1997) 153
- Muñoz-Caro, C., A. Niño and M.L. Senent, Theoretical study of the effect of torsional anharmonicity on the thermodynamic properties of methanol 273 (1997) 135
- Neufeld, A.A., P.A. Purtov and A.B. Doktorov, A novel representation in the CIDEP theory 273 (1997) 311
- Nguyen, M.T., see Creve, S. 273 (1997) 199
- Nielsen, N.C., see Hohwy, M. 273 (1997) 297
- Niño, A., see Muñoz-Caro, C. 273 (1997) 135
- Noguchi, T., see Cha, Y.-H. 273 (1997) 159
- Ohnishi, T., see Cha, Y.-H. 273 (1997) 159
- Parrinello, M., see Marx, D. 273 (1997) 360
- Petelenz, P., Degenerate Frenkel exciton states in the electroabsorption spectroscopy of molecular crystals 273 (1997) 42

- Piccirillo, S., see Douin, S. 273 (1997) 389
- Polyansky, O.L., see Prosimi, R. 273 (1997) 107
- Prosimi, R., O.L. Polyansky and J. Tennyson, A global potential energy surface for the H_3^+ molecule 273 (1997) 107
- Purtov, P.A., see Neufeld, A.A. 273 (1997) 311
- Rachlew-Källne, E., see Erman, P. 273 (1997) 239
- Ramaraj, R., see Retna Raj, C. 273 (1997) 285
- Rasing, T., see Jongma, R.T. 273 (1997) 147
- Reid, I.D., see Cox, S.F.J. 273 (1997) 179
- Reininger, R., see Al-Omari, A.K. 273 (1997) 402
- Reisch, H., see Rumi, M. 273 (1997) 429
- Retna Raj, C. and R. Ramaraj, γ -Cyclodextrin induced intermolecular excimer formation of thioflavin T 273 (1997) 285
- Richardi, J., H. Krienke and P.H. Fries, Dielectric constants of liquid formamide, N-methylformamide and dimethylformamide via molecular Ornstein-Zernike theory 273 (1997) 115
- Rieder, K.-H., see Bartels, L. 273 (1997) 371
- Rubio, A., see Marcos, P.A. 273 (1997) 367
- Rumi, M., G. Zerbi, U. Scherf and H. Reisch, Raman intensities and molecular hyperpolarizability of polyindenofluorene 273 (1997) 429
- Sangaletti, L., The effect of ligand correlations on the one-electron removal valence band of NiO 273 (1997) 279
- Sannes, P., see Erman, P. 273 (1997) 239
- Scherf, U., see Rumi, M. 273 (1997) 429
- Schoen, M. and D.J. Diestler, Liquid-vapor coexistence in a chemically heterogeneous slit-nanopore. Erratum. 273 (1997) 296
- Schrivier, A., see Bahou, M. 273 (1997) 31
- Schrivier-Mazzuoli, L., see Bahou, M. 273 (1997) 31
- Schröder, D., see Harvey, J.N. 273 (1997) 164
- Schwartz, R.L., D.T. Anderson, M.W. Todd and M.I. Lester, Infrared spectroscopy of OH-H₂ entrance channel complexes 273 (1997) 18
- Schwarz, H., see Harvey, J.N. 273 (1997) 164
- Senent, M.L., see Muñoz-Caro, C. 273 (1997) 135
- Sepiol, J., J. Jasny, J. Keller and U.P. Wild, Single molecules observed by immersion mirror objective. The orientation of terrylene molecules via the direction of its transition dipole moment 273 (1997) 444
- Sepiol, J., see Jasny, J. 273 (1997) 439
- Shaik, S., see Harvey, J.N. 273 (1997) 164
- Shao, L., N.J. Tao and R.M. Leblanc, Probing the microelastic properties of nanobiological particles with tapping mode atomic force microscopy 273 (1997) 37
- Shizuka, H., see Itoh, T. 273 (1997) 397
- Smith, S.C., see Jeffrey, S.J. 273 (1997) 55
- Soep, B., see Lopez-Martens, R. 273 (1997) 219
- Solgadi, D., see Lopez-Martens, R. 273 (1997) 219
- Song, M.-B., see Honda, Y. 273 (1997) 141
- Sorai, M., see Kawamura, T. 273 (1997) 235
- Spiess, H.W., see Hubrich, M. 273 (1997) 259

- Sprik, M., see Marx, D. 273 (1997) 360
- Stangassinger, A., see Knight, A.M. 273 (1997) 265
- Stankiewicz, M., see Erman, P. 273 (1997) 239
- Stass, D.V., see Tadjikov, B.M. 273 (1997) 25
- Steffen, T. and K. Duppen, Analysis of nonlinear optical contributions to temporally two-dimensional Raman scattering 273 (1997) 47
- Sun, Z., see Barnett, R.N. 273 (1997) 321
- Syage, J., see Lopez-Martens, R. 273 (1997) 219
- Tadjikov, B.M., D.V. Stass, O.M. Usov and Yu.N. Molin, MARY-detected ESR spectrum of solvent radical cations (holes) in squalane 273 (1997) 25
- Tao, N.J., see Shao, L. 273 (1997) 37
- Tappero, R., P. D'Arco and A. Lichanot, Electronic structure of α -MnS (alabandite): an ab initio study 273 (1997) 83
- Tasumi, M., see Cha, Y.-H. 273 (1997) 159
- Tatewaki, H., see Hashimoto, T. 273 (1997) 345
- Tennyson, J., see Prosmitti, R. 273 (1997) 107
- Thiel, W., see Dressler, S. 273 (1997) 71
- Todd, M.W., see Schwartz, R.L. 273 (1997) 18
- Tokue, I. and T. Ibuki, Photoabsorption cross sections and radiative processes of SnCl_4 and $\text{Sn}(\text{CH}_3)_4$ in the 6–31 eV region 273 (1997) 247
- Tozer, D.J., N.C. Handy and W.H. Green, Exchange-correlation functionals from ab initio electron densities 273 (1997) 183
- Usov, O.M., see Tadjikov, B.M. 273 (1997) 25
- Vager, Z., Experimentally realizable insight into the dynamics of chiral molecules 273 (1997) 407
- Vainer, Yu.G., see Zilker, S.J. 273 (1997) 232
- Veseth, L., see Erman, P. 273 (1997) 239
- Wang, D., J.Z.H. Zhang and C.-h. Yu, Quantum calculation of photodetachment spectrum of $\text{OH}^-(\text{H}_2)$ 273 (1997) 171
- Wang, W.-N., K.-N. Fan and S. Iwata, Ab initio MO studies of Si_4NO^+ clusters 273 (1997) 337
- Watanabe, A., T. Kodaira and O. Ito, Time-resolved emission spectra of poly(3-octylthiophene): energy migration in the π -conjugated polymer chain 273 (1997) 227
- Webster, B.C., see Cox, S.F.J. 273 (1997) 179
- Wild, U.P., see Sepiol, J. 273 (1997) 444
- Witschel, W. and C. Hartwigsen, Partition function and the level density of the hindered rotor 273 (1997) 304
- Yamaji, M., see Itoh, T. 273 (1997) 397
- Yamaki, T., K. Asai and K. Ishigure, RBS analysis of Langmuir–Blodgett films bearing quantum-sized CdS particles 273 (1997) 376
- Yassen, M., see Lifshitz, E. 273 (1997) 381
- Yoshiki Franzén, K., see Erman, P. 273 (1997) 239
- Yu, C.-h., see Wang, D. 273 (1997) 171
- Yu, M. and M. Dolg, Covalent contributions to bonding in group 12 dimers M_2 ($\text{M} = \text{Zn}, \text{Cd}, \text{Hg}$) 273 (1997) 329
- Yuan, J., see Zhang, X. 273 (1997) 416

- Zacharias, H., see Jongma, R.T. 273 (1997) 147
- Zerbi, G., see Rumi, M. 273 (1997) 429
- Zhang, J.Z.H., see Wang, D. 273 (1997) 171
- Zhang, X., J. Yuan, X. Liu, J.P. Jouart and G. Mary, Three-photon upconversion in Er^{3+} doped $\text{Ca}_3\text{Al}_2\text{Ge}_3\text{O}_{12}$ 273 (1997) 416
- Zilker, S.J., D. Haarer and Yu.G. Vainer, Line broadening mechanisms in spectra of organic amorphous solids: photon echo study of terrylene in polyisobutylene at sub-kelvin temperatures 273 (1997) 232